1-Methylpyrene

2381-21-7 | DTXSID0025654

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 107000 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.13e-01

Confidence level: 7.49e-01

Nearest Neighbors from the Training Set

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Pyrene
Measured: 79400
Predicted: 92600

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Fluoranthene
Measured: 63100
Predicted: 85300

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Benz(a)anthracene
Measured: 200000
Predicted: 227000

Image not found

Naphthacene
Measured: 646000
Predicted: 229000

Image not found

Benz[a]acridine
Measured: 24500
Predicted: 154000